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Study on Exposure Assessment Model of Dioxane in Shampoo

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Abstract

Setting dioxane in shampoo as the research object, exposure assessment of dioxane via skin route was studied. Scene simulation of dioxane exposure to human via skin was made after analysis of dioxane damage characteristics. Then the exposure assessment model of dioxane in shampoo via skin route was established and the concentration of dioxane was measured. The result shows that the concentration of dioxane is 7.213mg/kg when the confidence level reaches to 95%, average daily absorbed dose is 9.913×10^{-7}mg/(kg·d) and the cancer risk level of dioxane is 2.8914×10^{-7}/a.

Keywords: Shampoo, Dioxane, Exposure assessment, Model

Introduction

The shampoo has already become the essential articles for daily use. However, generally speaking, there is dioxane in shampoo, which is carcinogenic. The dioxane could penetrate into human body through skin, causing anesthesia and stimulation, and would accumulate in the human body, do harm to liver and skin, even cause uremia [1-2]. People who use shampoo containing dioxane would suffer tremendous harm. Although the Cosmetics health standards forbid the use of dioxane as the raw material for cosmetic, the dioxane is still the by-product in the production of shampoo, bath foam, liquid soap, and so on, due to the current technical factor. So it is highly important to evaluate the risks of harmful materials in these products.

Because of the lack of risk evaluation on chemical materials in products made in china, it is impossible for people to make sure which materials are hazards, of what quantity can they cause harm, and how much damage they can make. As the core process of risk evaluation, exposure evaluation on chemical materials is the focus of scholars' research.

For the process of the human body exposed to dioxane by skin, the real scene was simulated in this paper, the exposure evaluation model was established, and the exposure dose was finally calculated based on the analysis of the dioxane content in shampoo from the sample collected.

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1. Exposure scene simulation

The exposure of dioxane in shampoo on the human body mainly occurs during the process of washing hair. The access of dioxane is shampoo. Dioxane penetrates into human body through the contact of shampoo on the skin. When we wash our hair, the shampoo is poured out on the hand, and is smeared on the head. The position which has direct contact with human body is hand and the head skin. The head skin is more sensitive, and the dioxane on it would do more harm to human body. In contrast, the hand skin is less sensitive. So we only consider the exposure of head skin. In conclusion, the main contact part of human body, which is exposed to the dioxane is the head skin, and the medium is shampoo. The major factors affecting the exposure of dioxane on human body are the length of hair, the time of washing hair, the frequency of washing hair, and the amount of shampoo usage.

The harmful substances would be intercepted by protection barrier of human body when they penetrate into the skin, and the interception would stop large scale of harmful substances. As a result, every phase of exposure pathways should be confirmed in calculating the dosage in the exposure evaluation, and the amount of harmful substances should be calculated according to the particular case of every stage. The relation between the exposure pathways via skin and the amount is as the Fig. 1 shows.

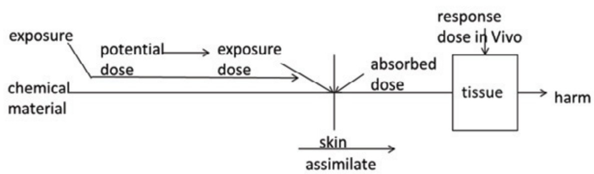


Fig.1.the exposure pathways via skin

2. Establishment of skin-exposure model

2.1. Identification of exposure factors

Once the values of exposure factors determined, the extent of exposure evaluation will be acquired, such as mean value, the maximum value and the boundary estimation. For example, the following formula should be adopted when calculating the LADD [3].

LADD=（the amount of chemical substance ×uptake rates ×the exposure time）/（the weight of human body× the average lifetime）

In the above formula, the variables could be seemed as the exposure factors, except the amount of chemical substances. Every exposure factors involves the characteristics of crowds, including the physical characteristics and the behavioral characteristics. For the process of dioxane exposure via skin, the exposure factors include the skin absorption coefficient, the weight of human body, and the area of head skin:

(1) absorption coefficient K_p

The exposure pathway via skin is relatively complex. The harmful substances which have contact with skin could not completely penetrate in human body. Instead, part of harmful substances which are filtrated by skin could enter into human body. So a parameter of the skin absorption degree is involved, which is called the skin absorption parameter. Through analysis, the model of skin absorption parameter is obtained as follows:

$$\log K_p = 0.71 \log K_{ow} - 0.0061 MW - 6.3 \tag{1}$$

Where, K_P—skin absorption parameter, cm/sec；

K_{OW}—octanol/water partition coefficient；

MW—chemical molecular mass.

(2) The weight of human body

The weight of human body is affected in many different ways, and the height is the major factor to the weight. In addition, the geographic diversity has great influence on the weight. The weight adopted in the risk evaluation is the standard weight. When Height>165cm: standard weight （kg） = height （cm） -100; When height <165cm: standard weight （kg） = height （cm） -105（male）.

Through the height measurement of male and female, age between 20 and 25, in all provinces(including Hong Kong, Macau and Taiwan), the average height of adult is calculated, that is even height of men is 171.78cm, and 161.87cm of women.

(3) Head area

The method of measurement and result of measurement statistics are given in the national standard head-face dimensions of adults [4]. The calculation model could be established by analyzing the measurement project:

$$S_h = 2KL^2/\pi \tag{2}$$

Where, K—Correction factor, usually value of 0.9;

L—Arc length between hairline and hair end point （L= hem width from crown to back point of low chin—Facial length I—Length of Antilobium-gnathion）.

Domestic man and woman head area test items required size statistics as is shown in table 1:

Table 1.Human size of facial and head

Gender	Project name	Mean （cm）	Standard deviation	Percentile 5	50	95
Male	Hem width from crown to back point of low chin	671	15.4	645	671	696
	Facial length I	190	5.94	180	190	200
	Length of Antilobium-gnathion	142	3.37	137	142	148
Female	Hem width from crown to back point of low chin	647	15.49	622	647	673
	Facial length I	176	5.83	167	176	186
	Length of Antilobium-gnathion	138	3.82	131	138	144

2.2. Establishment of exposure calculation model

The shampoo should be smeared on the head, but the head needs to be wetted before. So the form of shampoo has changed from liquid to foam, and the shampoo in the foam form has a definite volume. In addition, the concentration of harmful substances also has changed. So the diluted concentration of harmful substances should be accurately calculated to make sure the exposure situation of harmful substances. On such condition, the quantity of harmful substances (D_{der}) which the human body absorbs finally and responding daily average absorbance dosage (ADD_{int}) could be represented as below:

$$D_{der} = C_{der} \cdot K_p \cdot SA \cdot ED \tag{3}$$

$$ADD_{\mathrm{int}} = \frac{C_{der} \cdot K_p \cdot SA \cdot ED}{BW \cdot AT} \tag{4}$$

Where, C_{der}—concentration of dioxane in shampoo, mg/L;

K_p—absorption coefficient via skin, cm/h;

SA—Skin contact area, cm^2;

ED—Exposure time, h;

BW—human weight, kg;

AT—weighted exposure time, day.

The exposure evaluation of harmful substances in shampoo is relatively cumbersome. The shampoo will be convert bubble in the presence of water, as a result, the volume of shampoo and the concentration of harmful material will change correspondingly. The types of foaming agent and content are not identical in different shampoo, which lead uncertainty of shampoo volume when used. Expansion coefficient or dilution factor can be introduced for this kind of situation, then the concentration of harmful substance in the diluted products can be approximately estimated.

3. Application case

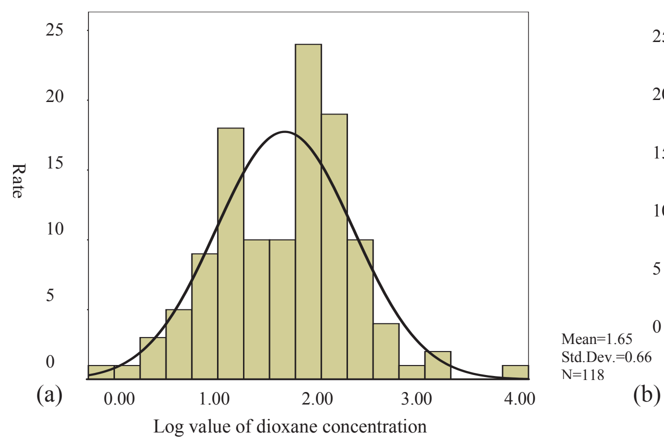
3.1. Data analysis

The quantitative detection of dioxane was determined with the method of gas chromatography - mass spectrometry on the cosmetics samples collected from domestic brand of more than 118 samples, and the test results can be seen in table 2.

Table 2.Test result of dioxane

Sample number	Dioxane content (mg/kg)	Sample number	Dioxane content (mg/kg)	Sample number	Dioxane content (mg/kg)
1	<2.50	12	<2.50	23	6.34
2	<2.50	13	<2.50	24	6.31
3	11.04	14	3.33	25	4.9
4	21.64	15	13.54	26	10.44
5	<2. 50	16	18.04	27	9.74
6	4.61	17	47.93	28	9.35
7	3.53	18	3.62	29	8.89
8	4.43	19	3.23	30	8.25
9	10.15	20	2.84	31	7.69
10	13.75	21	6.48	32	7.53
11	<2.5	22	13.09	33	8.87

The concentration of dioxane was determined by SPSS, and the test results of logarithm value are statistical analyzed with the method of histogram and box chart, results are as shown in Fig.2.



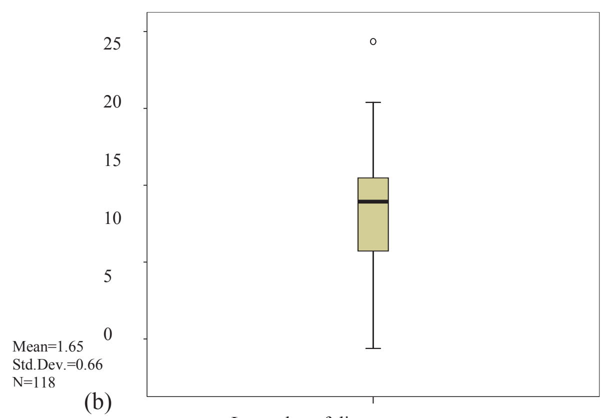


Fig.2.Test results of the numerical histogram (a), and the numerical stem figure(b)

It can be seen from histogram figure that the whole data obeys normal distribution trend and data stability is good from stem figure. The partial degree and the kurtosis U value of data that obeys normal distribution are calculated as 0.156 and 0.846, all of which are less than 1.96, that is P>0.05. It can be concluded that the log value of dioxane fit normal distribution.

In order to further analysis the extend that test results fit normal distribution, Kolmogorov-Smirnov method and Shapiro-Wilk method are used to verify its normal distribution. Shapiro-Wilk statistics are calculated with SPSS software, and results show that the significant level is $p=0.190>0.05$. Finally, we can draw a conclusion that residual volume quantity of dioxane fit normal distribution, and the mean value is 6.469, variance is 23.14.

3.2. Set the exposure scenario

The frequency of men washing his hair is between once every three days and one time per day. It is different due to the difference of geography and lifestyle. Based on the principle of injury maximizing, it is assumed that men's shampoo frequency is once a day in this paper. The law of shampoo time is as follows: 3 to 5 minutes for scrubbing, 2 to 3 minutes for rinsing and the total time of shampoo is 5 to 8 minutes.

Set the scene: A normal male adult, 24 years old, height of 171.78cm, washes his hair at home. Airflow disrupting is small. He uses a kind of ordinary shampoo, of which dioxane concentration is 1.3g/ml (the average concentration of shampoo) and scrubs for 5 minutes.

3.3. Calculation of dioxane exposure dose

(1) Dioxane concentration C_{der}

The measured unit of dioxane concentration is mg / kg. The dioxane concentration is 9.377mg / L by converting the measured unit.

(2) Human body weight BW

By bring height 171.78 into the standard weight formula based on the male: male body weight (kg) = height (cm) -100, it is drawn that body weight is 71.78kg.

(3) Absorption coefficient through skin K_p

By bring dioxane octanol-water absorption coefficient -0.27 and the molecular weight 88.11 into the equation (1), it is drawn that dioxane absorption coefficient through skin K_p is 3.366×10^{-4}cm / h.

(4) Contact area between the skin and shampoo S_h

When each parameter using the 95% percentile value, L=696-200-148=348(cm). By bring L into the equation (2), it is drawn that the human head area is $0.0694m^2$.

(5) Dilution factor D

Value of dilution factor is between 0-1. It is different due to characteristics of product. Based on the principle of injury maximizing, the dilution factor is 1 in this paper when calculating the exposure dose of dioxane in shampoo.

(6) Exposure time

5 minutes a day, that is 1/12h.

(7) Absorbed dose for human exposure to dioxane

It is drawn that the absorbed dose of lifetime exposure to dioxane is 46.452mg by bring the above factors' value into the formula (3). Daily average absorbed dose is mg / (kg·d) by bring the factors into formula (4).

This paper focuses on the carcinogenic effects of dioxane. There is an international unified formula of the level of cancer risk. Carcinogenic risk is generally in terms of life-long exposure of the human body against harmful substances. Chemicals carcinogenic risk level P is calculated as follow: $P=1-exp(-q\times LADD)$, where, q is the carcinogenicity of chemicals coefficient. LADD is the average daily exposure dose of chemicals in the life. The carcinogenicity strength coefficient of dioxane is 0.2917 (kg·d) / mg. Cancer risk level of dioxane in shampoo is calculated to be 2.8914×10^{-7} / a. The maximum acceptable level of risk of carcinogenic chemicals is 1×10^{-6} /a in Britain, the Netherlands and other countries. The U. S. requires that the maximum acceptable level of risk of carcinogenic chemicals is 1×10^{-4} / a. Therefore, the level of carcinogenic risk of dioxane in shampoo is in the acceptable range.

4. Summary

The exposure process of dioxane via skin route is determined by analyzing the injury scene that dioxane in Shampoo exposing to the human body via skin, and a model of dioxane exposure via skin is established. By applying this model to specific examples, it is drawn that the lifetime absorbed dose of dioxane is 46.452mg and average daily absorbed dose is 9.913×10^{-7}mg / (kg·d), and the dioxane cancer risk level is 2.8914×10^{-7}/ a. By comparison, it is determined that the cancer risk level of dioxane in shampoo is in the acceptable range.

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